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EDUCATION

- 8/85 Ph.D. in Physics, College of William and Mary in Virginia.
Thesis: First-Principles Structure Calculations Using the General Potential LAPW Method
Advisor: Professor Henry Krakauer
- 5/83 M.S. in Physics, College of William and Mary in Virginia.
- 6/81 B.S. in Physics, Fudan University, Shanghai, China.

WORK EXPERIENCE

- 4/03 to present
Principal Scientist (04/03) and Team Leader, Computational Materials Science Group,
National Renewable Energy Laboratory (NREL) (formerly SERI).
- 4/95 to 3/03
Senior Scientist II and Team Leader (since 10/99), NREL.
- 4/92 to 3/95
Senior Scientist I, NREL.
- 1/90 to 3/92
Staff Scientist, NREL.
- 8/85 to 12/89
Postdoctoral Researcher/Research Associate, Solar Energy Research Institute (SERI).
- 8/83 to 8/85
Graduate Research Assistant, College of William and Mary.
Research Subject: Electronic structure theory. Advisor: Prof. Henry Krakauer.
- 8/82 to 8/83
Graduate Research Assistant, College of William and Mary.
Research Subject: Muon spin resonance. Advisor: Prof. Kenneth G. Petzinger.
- 8/81 to 8/82
Teaching Assistant, Department of Physics, College of William and Mary.
- 12/75 to 2/78
Mathematics Teacher, Technical School Affiliated to Shanghai Plastic Research Institute.

AREAS OF SPECIALIZATION

Professional Skills

Strong background in solid state theory, computer modeling, and large scale numerical simulation.

Scientific Achievements

Developed a completely general, full potential, self-consistent LAPW code for electronic structure and total energy calculations. Made original and significant contributions to the understanding of (i) electronic structures and stabilities of semiconductor and metallic alloys, superlattices, surfaces, and filled-tetrahedron compounds; (ii) effect of d and f electrons in II-VI and magnetic semiconductors; (iii) chemical trends of band offsets and pressure coefficients of semiconductors; (iv) electronic structures of wide band gap nitrides and oxides; (v) defect physics in semiconductors and insulators; and (vi) electronic structure of nano, organic, and hybrid semiconductors.

Languages:

Fluent in English and Chinese.

Publications and Presentations:

More than 210 peer-reviewed publications, including more than 50 papers in **Physical Review Letters** and **Physical Review Rapid Communications**, and more than 6200 citations. 18 of the papers have more than 100 citations and more than 45 of the papers have more than 50 citations. Presented many invited talks in international conferences.

Some of the recent invited talks are:

“Overcoming the doping bottleneck in semiconductors and Insulators”, International Conference on Materials for Advanced Technologies (ICMAT2003), Singapore, December 7-12, 2003.

“Theory of Multinary compounds: Challenges for the theorists and experimentalists”, 14th International Conference of Ternary and Multinary Compounds, Denver, Colorado, September 27 - October 1, 2004.

“Theoretical investigation of the InN Band Gap Anomaly”, The European Materials Research Society 2005 Fall Meeting, Warsaw, Poland, September 5-9, 2005.

Professional Membership:

American Physical Society, Materials Research Society

HONORS AND AWARDS

Chunky Bullet Award, DOE/BES 2002

Outstanding Performance Award, NREL, 2001

Fellow of American Physical Society, 1999

Outstanding Researcher Award, DOE, 1995

Graduate Student Fellowship, College of William and Mary, 1981 - 1985

Winner of the CUSPEA (China-U.S. Physics Education and Application), 1981

PUBLICATIONS

Numbers in [] is the citation number according to ISI on October 1, 2005

- (1) “Zero field muon spin depolarization revisited”, K. G. Petzinger and **S.-H. Wei**, *Hyperfine Interaction* **17-19**, 441 (1984).[1]
- (2) “Local-density-functional calculation of the pressure-induced metalization of BaSe and BaTe”, **S.-H. Wei** and H. Krakauer, *Phys Rev. Lett.* **55**, 1200 (1985).[366]
- (3) “Linearized augmented-plane wave calculation of the electronic structure and total energy of tungsten”, **S.-H. Wei**, H. Krakauer, and M. Weinert, *Phys. Rev. B* **32**, 7792 (1985).[96]
- (4) “Instability of the ideal tungsten (001) surface”, D. Singh, **S.-H. Wei**, and H. Krakauer, *Phys. Rev. Lett.* **57**, 3292 (1986).[43]
- (5) “Electronic structure and phase stability of LiZnAs: A half ionic and half covalent tetrahedral semiconductor”, **S.-H. Wei** and A. Zunger, *Phys. Rev. Lett.* **56**, 528 (1986).[27]
- (6) “Alloy-stabilized semiconducting and magnetic zinc-blende phase of MnTe”, **S.-H. Wei** and A. Zunger, *Phys. Rev. Lett.* **56**, 2391 (1986).[51]
- (7) “Thermodynamic instability of ultrathin semiconductor superlattices”, D.M. Wood, **S.-H. Wei**, and A. Zunger, *Phys. Rev. Lett.* **58**, 1123 (1987).[50]
- (8) “Total energy and band structure calculation for the semimagnetic $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ semiconductor alloy and its binary constituents”, **S.-H. Wei** and A. Zunger, *Phys. Rev. B* **35**, 2340 (1987).[156]
- (9) “Phase stability and band structure of the semimagnetic $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ semiconductor alloy”, **S.-H. Wei** and A. Zunger, in *Ternary and Multinary Compounds*, edited by S. K. Deb and A. Zunger, (Material Research Society, Pittsburgh, 1987), p.485.
- (10) “Electronic structure and stability of $\text{A}^{\text{I}}\text{B}^{\text{II}}\text{C}^{\text{V}}$ filled tetrahedral compounds”, D. M. Wood, **S.-H. Wei**, and A. Zunger, in *Ternary and Multinary Compounds*, edited by S. K. Deb and A. Zunger, (Material Research Society, Pittsburgh, 1987), p. 523.
- (11) “Band structure and electronic excitations in $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ ”, **S.-H. Wei** and A. Zunger, in *Diluted Magnetic (Semimagnetic) Semiconductors*, edited by J. K. Furdyna, R. L. Aggarwal, and S. von Molnar (Material Research Society, Pittsburgh, 1987), p. 197 (1987).
- (12) “Common-anion rule and its limits: photoemission studies of $\text{CuIn}_x\text{Ga}_{1-x}\text{Se}_2\text{-Ge}$ and $\text{Cu}_x\text{Ag}_{1-x}\text{InSe}_2\text{-Ge}$ interfaces”, D. G. Kilday, G. Margaritondo, T. F. Ciszek, S. K. Deb, **S.-H. Wei** and A. Zunger, *Phys. Rev. B* **36** (**Rapid Communication**), 9388 (1987).[9]
- (13) “Electronic structure of $\text{M}_3^{\text{I}}\text{Sb}$ -type filled tetrahedral semiconductors”, **S.-H. Wei** and A. Zunger, *Phys. Rev. B* **35**, 3952 (1987).[5]
- (14) “Role of d orbital in valence band offsets of common-anion semiconductors”, **S.-H. Wei**, and A. Zunger, *Phys. Rev. Lett.* **59**, 144 (1987).[122]

- (15) "Comment on 'Coulomb energy in pseudobinary alloys' ", **S.-H. Wei**, *Phys. Rev. Lett.* **59**, 2613 (1987).[7]
- (16) "Calculation of the valence band offsets of common-anion semiconductor heterojunctions from core levels: the role of cation d orbital", **S.-H. Wei** and A. Zunger, *J. Vac. Sci. & Technol. B* **5**, 1239 (1987).[16]
- (17) "First-principles calculations of the phase diagrams of noble metals: Cu-Au, Cu-Ag and Ag-Au", **S.-H. Wei**, A. A. Mbaye, L. G. Ferreira, and A. Zunger, *Phys. Rev. B* **36**, 4163 (1987).[74]
- (18) "The solution of large dense generalized eigenvalue problems on the Cray X-MP/24 with SSD", G. Roger, H. Krakauer, J. Lewis, H. Simon, and **S.-H. Wei**, *J. Comput. Phys.* **69**, 471 (1987).[3]
- (19) "Stability and electronic structure of ultrathin [001] $(\text{GaAs})_m(\text{AlAs})_m$ superlattices", D. M. Wood, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **37**, 1342 (1988).[50]
- (20) "Ordering-induced changes in the optical spectra of semiconductor alloys", J. E. Bernard, **S.-H. Wei**, D. M. Wood, and A. Zunger, *Appl. Phys. Lett.* **52**, 311 (1988).[28]
- (21) "A novel viewpoint on the Cu-Au phase diagram: the interplay between fixed Ising energies and elastic effects", A. Zunger, **S.-H. Wei**, A. A. Mbaye, and L. G. Ferreira, *Acta Metall.* **36**, 2239 (1988).[17]
- (22) "Electronic structure of II-VI compounds and their alloys: role of cation d bands", **S.-H. Wei** and A. Zunger, *J. Crystal Growth* **86**, 1 (1988).[8]
- (23) "Role of metal d states in II-VI semiconductors", **S.-H. Wei** and A. Zunger, *Phys. Rev. B* **37**, 8958 (1988).[182]
- (24) "Electronic structure of ultrathin $(\text{GaAs})_n(\text{AlAs})_n$ [001] superlattices and the $\text{Ga}_{0.5}\text{Al}_{0.5}\text{As}$ alloy", **S.-H. Wei**, and A. Zunger, *J. Appl. Phys.* **63**, 5794 (1988).[62]
- (25) "Electronic structure and stability of II-VI semiconductors and their alloys: the role of metal d bands", **S.-H. Wei** and A. Zunger, *J. Vac. Sci. & Technol. A* **6**, 2597 (1988).[43]
- (26) "Ordering of isovalent intersemiconductor alloys", J. E. Bernard, L. G. Ferreira, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **38** (**Rapid Communication**), 6338 (1988).[65]
- (27) "Thermodynamic stability of $(\text{AlAs})_n(\text{GaAs})_n$ superlattices and the random $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$ alloy", **S.-H. Wei** and A. Zunger, *Phys. Rev. Lett.* **61**, 1505 (1988).[30]
- (28) "(111)-oriented $(\text{GaAs})_n(\text{AlAs})_n$ superlattices are direct band-gap materials for all n 's" **S.-H. Wei** and A. Zunger, *Appl. Phys. Lett.* **53**, 2077 (1988).[20]
- (29) "Epitaxy-induced structural phase transformations", S. Froyen, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **38** (**Rapid Communication**), 10124 (1988).[45]
- (30) "First-principles calculation of alloy phase diagrams: the renormalized interaction approach", L. G. Ferreira, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **40**, 3197 (1989).[108]

- (31) "Band gaps and spin-orbit splitting of ordered and disordered $\text{Al}_{1-x}\text{Ga}_x\text{As}$ and $\text{GaAs}_x\text{Sb}_{1-x}$ alloys", **S.-H. Wei** and A. Zunger, *Phys. Rev. B* **39**, 3279 (1989).[158]
- (32) "Negative spin-orbit bowing in semiconductor alloys", **S.-H. Wei** and A. Zunger, *Phys. Rev. B* **39 (Rapid Communication)**, 6279 (1989).[13]
- (33) "First-principles calculation of the formation energies of ordered and disordered phases of AlAs-GaAs ", N. E. Christensen, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **40**, 1642 (1989).[12]
- (34) "First-principles theory of alloy phase diagram", A. Zunger, L. G. Ferreira, and **S.-H. Wei**, in *Atomic Scale Calculations in Material Science*, edited by J. Tersoff, D. Vanderbilt, and V. Vitek, (Material Research Society, Pittsburgh, 1989), p. 177.
- (35) "Instability of diatomic deuterium in fcc palladium", **S.-H. Wei** and A. Zunger, *J. Fusion Energy* **9**, 367 (1990).[2]
- (36) "Absence of volume metastability in bcc copper", Z. W. Lu, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **41**, 2699 (1990).[24]
- (37) "Stability of coherently strained semiconductor superlattices", R. G. Dandrea, J. E. Bernard, **S.-H. Wei**, and A. Zunger, *Phys. Rev. Lett.* **64**, 36 (1990).[55]
- (38) "Band gap narrowing in ordered and disordered semiconductor alloys", **S.-H. Wei** and A. Zunger, *Appl. Phys. Lett.* **56**, 662 (1990).[179]
- (39) "Stability of atomic and diatomic hydrogen in fcc palladium", **S.-H. Wei** and A. Zunger, *Solid State Commun.* **73**, 327 (1990).[5]
- (40) "First-principles calculation of temperature-composition phase diagrams of semiconductor alloys", **S.-H. Wei**, L. G. Ferreira, and A. Zunger, *Phys. Rev. B* **41**, 8240 (1990).[124]
- (41) "Special quasirandom structure", A. Zunger, **S.-H. Wei**, L. G. Ferreira, and J. E. Bernard, *Phys. Rev. Lett.* **65**, 353 (1990).[137]
- (42) "Ordering in semiconductor alloys", J. E. Bernard, R. G. Dandrea, L. G. Ferreira, S. Froyen, **S.-H. Wei**, and A. Zunger, *Appl. Phys. Lett.* **56**, 731 (1990).[29]
- (43) "Electronic properties of random alloys: special quasirandom structures", **S.-H. Wei**, L. G. Ferreira, J. E. Bernard, and A. Zunger, *Phys. Rev. B* **42**, 9622 (1990).[96]
- (44) "Ground state structures and the random state energy of the Madelung lattice", R. Magri, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **42 (Rapid Communication)**, 11388 (1990).[75]
- (45) "Stability, electronic structure and phase diagrams of novel inter-semiconductor compounds", L. G. Ferreira, **S.-H. Wei**, and A. Zunger, *Inter. J. Supercomp. Appl.* **5**, 34 (1991).[30]
- (46) "Pseudopotential plane-wave calculations for ZnS ", J. L. Martins, N. Troullier, and **S.-H. Wei**, *Phys. Rev. B* **43**, 2213 (1991).[80]
- (47) "Ground state structures of intermetallic compounds: a first-principles Ising model", Z. W. Lu, **S.-H. Wei**, and A. Zunger, *Solid State Commun* **78**, 583 (1991).[14]

- (48) “First-principles statistical mechanics of structural stability of intermetallic compounds”, Z. W. Lu, **S.-H. Wei**, A. Zunger, S. Frota-Pessoa, and L. G. Ferreira, *Phys. Rev. B* **44**, 512 (1991).[161]
- (49) “Disorder effects on the density of states of the II-VI semiconductor alloys $\text{Hg}_{0.5}\text{Cd}_{0.5}\text{Te}$, $\text{Cd}_{0.5}\text{Zn}_{0.5}\text{Te}$ and $\text{Hg}_{0.5}\text{Zn}_{0.5}\text{Te}$ ”, **S.-H. Wei** and A. Zunger, *Phys. Rev. B* **43**, 1662 (1991); *ibid.*, 14272 (1991).[60]
- (50) “Long-range order in binary late transition metal alloys”, Z. W. Lu, **S.-H. Wei**, and A. Zunger, **Phys. Rev. Lett.** **66**, 1753 (1991).[54]
- (51) “Electronic structure of random $\text{Ag}_{0.5}\text{Pd}_{0.5}$ and $\text{Ag}_{0.5}\text{Au}_{0.5}$ alloys”, Z. W. Lu, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **44**, 10470 (1991).[43]
- (52) “Proposal for new III-V structures with infrared band gaps”, **S.-H. Wei** and A. Zunger, *Appl. Phys. Lett.* **58**, 2684 (1991).[41]
- (53) “Large lattice-relaxation-induced electronic level shifts in random $\text{Cu}_{1-x}\text{Pd}_x$ alloys”, Z. W. Lu, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **44** (**Rapid Communication**), 3387 (1991).[30]
- (54) “Comment on origins of compositional order in NiPt alloys”, Z. W. Lu, **S.-H. Wei**, and A. Zunger, **Phys. Rev. Lett.** **68**, 1961 (1992).[19]
- (55) “Electronic structures of ordered and disordered Cu_3Au and Cu_3Pd ”, Z. W. Lu, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **45**, 10314 (1992).[57]
- (56) “First-principles calculation of order-disorder transition in chalcopyrite semiconductors”, **S.-H. Wei**, L. G. Ferreira and A. Zunger, *Phys. Rev. B* **45** (**Rapid Communication**), 2533 (1992).[38]
- (57) “Theory of bonding charge density in $\beta\text{-NiAl}$ ”, Z. W. Lu, **S.-H. Wei**, and A. Zunger, *Acta Metall. Mater.* **40**, 2155 (1992).[21]
- (58) “Evolution of alloy properties with long-range order”, D. B. Laks, **S.-H. Wei**, and A. Zunger, **Phys. Rev. Lett.** **69**, 3766 (1992).[61]
- (59) “Prediction of new low temperature structures using first-principles statistical mechanics”, A. Zunger, Z. W. Lu, **S.-H. Wei**, L. G. Ferreira, and S. Frota-Pessoa, in *Modern Topics of Condensed Matters*, edited by J. L. Heiras and T. Akachi (ETC, Morelos, Mexico, 1992), p. 147.
- (60) “Stability and metastability of semiconductor alloys”, L. G. Ferreira, A. Zunger, **S.-H. Wei**, Z. W. Lu, in *Semiconductor Physics*, edited by J. R. Leite, A. Fazzio, and A. S. Chaves, (World Scientific, Singapore, 1992), p. 42.
- (61) “Relativity-induced ordering and phase-separation in intermetallic compounds”, Z. W. Lu, **S.-H. Wei**, and A. Zunger, *Euro. Phys. Lett.* **21**, 221 (1993).[25]
- (62) “First-principles phase diagrams of pseudoternary chalcopyrite/zinc-blende alloys”, R. Osorio, Z. W. Lu, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **47** (**Rapid Communication**), 9985 (1993).[8]

- (63) “Off-center atomic displacements in zinc-blende semiconductor”, **S.-H. Wei**, S. B. Zhang, and A. Zunger, **Phys. Rev. Lett.** **70**, 1639 (1993).[28]
- (64) “Dependence of the optical properties of semiconductor alloys on the degree of long range order”, **S.-H. Wei**, D. B. Laks, and A. Zunger, *Appl. Phys. Lett.* **62**, 1937 (1993); *ibid* **63**, 1292 (1993).[105]
- (65) “Electronic origin of magnetic phase transition in zinc-blende Mn chalcogenides”, **S.-H. Wei** and A. Zunger, *Phys. Rev. B* **48**, 6111 (1993).[23]
- (66) “Electronic structure of II-VI semiconductor and their alloys”, **S.-H. Wei**, in *II-VI Semiconductor Compounds*, edited by M. Jain (World Scientific, Singapore, 1993), p. 71.
- (67) “Band offset at the CdS/CuInSe₂ heterojunction”, **S.-H. Wei** and A. Zunger, *Appl. Phys. Lett.* **63**, 2549 (1993).[20]
- (68) “Theoretical and experimental studies of the ZnSe/CuInSe₂ heterojunction band offset”, A. J. Nelson, C. R. Schwerdtfeger, **S.-H. Wei**, A. Zunger, D. Rioux, R. Patel, and H. Hochst, *Appl. Phys. Lett.* **62**, 2557 (1993).[13]
- (69) “Influence of Ga concentration on the ordering process of Ga_xIn_{1-x}P grown on GaAs”, A. Eyal, R. Beserman, **S.-H. Wei**, A. Zunger, E. Maayan, O. Kreinin, J. Salzman, R. Westphalen, and K. Heime, *Jpn. J. Appl. Phys. Suppl.* **32-3**, 716 (1993).[6]
- (70) “Structural instability in zinc-blende semiconductors”, **S.-H. Wei**, S. B. Zhang, and A. Zunger, *Ferroelectrics*, **155**, 127 (1994).[]
- (71) “Prediction and observation of II-VI/CuInSe₂ heterojunction band offsets”, A. J. Nelson, D. W. Niles, C. R. Schwerdtfeger, **S.-H. Wei**, A. Zunger, and H. Hochst, *J. Electron Spectro. and Relat. Phenol.* **68**, 185 (1994).[10]
- (72) “Optical properties of zinc-blende semiconductor alloys: effects of epitaxial strain and chemical ordering”, **S.-H. Wei** and A. Zunger, *Phys. Rev. B.* **49**, 14337 (1994).[86]
- (73) “Strain effects on the spectra of spontaneously ordered Ga_xIn_{1-x}P”, **S.-H. Wei** and A. Zunger, *Appl. Phys. Lett.* **64**, 757 (1994).[18]
- (74) “Optical anisotropy and spin polarization in ordered GaInP”, **S.-H. Wei** and A. Zunger, *Appl. Phys. Lett.* **64**, 1676 (1994).[24]
- (75) “First principles simulated annealing study of phase-transition and short-range order in alloys”, Z. W. Lu, D. B. Laks, **S.-H. Wei** and A. Zunger, *Phys. Rev. B* **50**, 6642 (1994).[41]
- (76) “Relationships between the band gaps of the zinc-blende and wurtzite modifications of semiconductors”, C.-Y. Yeh, **S.-H. Wei** and A. Zunger, *Phys. Rev. B* **50 (Rapid Communication)**, 2715 (1994).[30]
- (77) “Type-II → type-I transition in (GaX)_n/(InX)_n (001) superlattices (X=P, Sb) as a function of period *n*”, A. Franceschetti, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **50 (Rapid Communication)**, 8094 (1994).[10]

- (78) “Absolute deformation potentials of Al, Si, and NaCl”, A. Franceschetti, **S.-H. Wei**, and A. Zunger, Phys. Rev. B **50**, 17797 (1994).[11]
- (79) “ E_1 , E_2 , and E'_0 transitions and pressure dependence in ordered $\text{Ga}_{0.5}\text{In}_{0.5}\text{P}$ ”, **S.-H. Wei**, A. Franceschetti, and A. Zunger, Phys. Rev. B **51**, 13097 (1995).[13]
- (80) “Theory of reflectance difference spectroscopy in ordered III-V semiconductor alloys”, **S.-H. Wei** and A. Zunger, Phys. Rev. B **51**, 14110 (1995).[10]
- (81) “Band offset and optical bowing of chalcopyrite and Zn-based II-VI alloys”, **S.-H. Wei** and A. Zunger, J. Appl. Phys. **78**, 3846 (1995).[72]
- (82) “Optical properties of $\text{Ga}_{0.5}\text{In}_{0.5}\text{P}$: Effects of strain and ordering”, **S.-H. Wei** and A. Zunger, in *Proceedings of the 22nd International Conference on the Physics of Semiconductors*, edited by D. J. Lockwood, (World Scientific, Singapore, 1995), p.1268.
- (83) “InAsSb/InAs: A type-I or a type-II band alignment”, **S.-H. Wei** and A. Zunger, Phys. Rev. B **52**, 12039 (1995).[22]
- (84) “Electronic structure theory of chalcopyrite alloys, interfaces, and ordered vacancy compounds”, A. Zunger and **S.-H. Wei**, in *Proceedings of the 13th NREL PV Program Review*, edited by H. S. Ullal and C. E. Witt, (AIP, New York, 1996), p.155.
- (85) “Effects of ordering on the electron effective mass and strain deformation potential in GaInP_2 : deficiencies of the k-p model”, A. Franceschetti, **S.-H. Wei** and A. Zunger, Phys. Rev. B **52**, 13992 (1995).[14]
- (86) “d-band excitations in II-VI semiconductors: A broken symmetry approach to the core hole”, S. B. Zhang, **S.-H. Wei** and A. Zunger, Phys. Rev. B **52**, 13975 (1995).[22]
- (87) “Giant and composition dependent optical bowing coefficient in GaAsN alloy”, **S.-H. Wei** and A. Zunger, **Phys. Rev. Lett.** **76**, 664 (1996).[254]
- (88) “Theoretical studies of chalcopyrite alloys, interfaces and ordered vacancy compounds”, **S.-H. Wei** and A. Zunger, Cryst. Res. Technol. **31**, 81 (1996).[]
- (89) “Fundamental optical transitions in GaN”, G.D. Chen, M. Smith, J. Y. Lin, H. X. Jiang, **S.-H. Wei**, M. A. Khan and C. J. Sun, Appl. Phys. Lett. **68**, 2784 (1996).[89]
- (90) “Chemical trends in band offsets of Zn and Mn-based II-VI’s: d-level pinning and offset compression”, **S.-H. Wei** and A. Zunger, Phys. Rev. B **53** (**Rapid Communication**), 10457 (1996).[14]
- (91) “Dependence of optical properties of semiconductor alloys on long range order, strain and pressure”, **S.-H. Wei**, A. Franceschetti and A. Zunger, in *Optoelectronic Materials - Ordering, Composition Modulation, and Self-Assembled Structures*, edited by E. D. Jones, A. Mascarenhas, and P. Petroff, (MRS, Pittsburgh, 1996), p.3.

- (92) “Prediction of new fingerprints of ordering in GaInP₂ alloys”, A. Franceschetti, **S.-H. Wei** and A. Zunger, in *Optoelectronic Materials - Ordering, Composition Modulation, and Self-Assembled Structures*, edited by E. D. Jones, A. Mascarenhas, and P. Petroff, (MRS, Pittsburgh, 1996), p.103.
- (93) “Point-charge electrostatics in disordered alloys”, C. Wolverton, A. Zunger, S. Froyen, and **S.-H. Wei**, *Phys. Rev. B* **54**, 7843 (1996).[17]
- (94) “Valence band splittings and band offsets of AlN, GaN and InN”, **S.-H. Wei** and A. Zunger, *Appl. Phys. Lett.* **69**, 2719 (1996).[104]
- (95) “Localization and percolation in semiconductor alloys: GaAsN vs GaAsP”, L. Bellaiche, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **54**, 17568 (1996).[155]
- (96) “Composition-dependence of interband transition intensities in semiconductor alloys: GaPN vs GaPAs”, L. Bellaiche, **S.-H. Wei**, and A. Zunger, *Phys. Rev. B* **56**, 10233 (1997).[79]
- (97) “Stabilization of ternary compounds via ordered array of defect pairs”, S. B. Zhang, **S.-H. Wei** and Alex Zunger, *Phys. Rev. Lett.* **78**, 4059 (1997).[59]
- (98) “Electronic and structural anomalies in lead chalcogenides”, **S.-H. Wei** and A. Zunger, *Phys. Rev. B* **55**, 13605 (1997).[28]
- (99) “Why is CuInSe₂ tolerant to defects and what is the origin of ordered defect structures”, A. Zunger, S. B. Zhang, and **S.-H. Wei**, in *Proceedings of the 14th NREL PV Program Review*, edited by C. E. Witt, (AIP, New York, 1997), p.63.
- (100) “Point-ion vs density functional calculations of electric field gradients in ordered GaInP₂”, **S.-H. Wei** and A. Zunger, *J. Phys. Chem.* **107**, 1931 (1997).[4]
- (101) “Band gaps of GaPN and GaAsN alloys”, L. Bellaiche, **S.-H. Wei** and A. Zunger, *Appl. Phys. Lett.* **70**, 3558 (1997).[89]
- (102) “Bond length distribution in tetrahedral vs octahedral semiconductor alloys: The case of GaInN”, L. Bellaiche, **S.-H. Wei** and A. Zunger, *Phys. Rev. B* **56**, 13872 (1997).[10]
- (103) “Why is heavily-defected CuInSe₂ a good opto-electronic material: Defect physics in CuInSe₂”, **S.-H. Wei**, S. B. Zhang, and A. Zunger, in *Proceedings of the 11th Inter. Conf. of Ternary and Multinary Compounds*, edited by R. D. Tomlinson, (AIP, New York, 1998), p. 765.[3]
- (104) “Spin polarization of photoelectrons from ordered semiconductor alloys”, **S.-H. Wei** in *Proceedings of the 7th Inter. Workshop on Polarized Gas Targets and Polarized Beams*, edited by R. J. Holt and M. A. Miller, (AIP, New York, 1998), p. 284.
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